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Background

The shortcomings of the classic low order and geometrically inflexible particle-in-cell methods for the modeling of kinetic plasma phenomena approach are also becoming increasing clear when one attempts to model many types of applications of mission critical importance to the US Airforce. However, the development of faster and more accurate alternatives remains a major challenge, since such developments require one to rethink fundamental choices and design criteria.

In this effort we have focused the research on the development of computational methods for the modeling of plasma problems dominated by kinetic effects and we consider methods where the spatial dimensions are discretized by using a Discontinuous Galerkin method. For the phase-space dynamics we primarily seek to develop a new generation of particle-in-cell methods for solving high-speed problems on general unstructured grids but we also consider challenges associated with efficiently solving the Vlasov equation. Applications include accelerators, microwave generators and laser-matter interaction.

While such methods have been successfully developed during beginning of this project, these techniques tend to be computationally very demanding. A significant part of the project is therefore also devoted to the development of new efficient algorithms and their efficient implementation on modern computational platforms.

In the latter part of the efforts we have begun to focus on the accurate modeling of complex continuum problems to lay the ground for the development of efficient and accurate hybrid method to enable the future modeling of complex multi-scale problems.

Overview of contributions.

Throughout the effort, we have pursed the development and analysis of a number of algorithms for kinetic plasma physics modeling.

Basic algorithms: We have developed and analysed novel and fast ways of identifying and depositing charge and currents to the nodes of the DG method in a PIC simulation. This step of the scheme was identified as the computational bottleneck and we developed and investigated several techniques, including ones exploring the use of a Cartesian grid as an intermediary between the charge deposition and the unstructured grids. The properties of these techniques in terms of charge, energy, and momentum conservation have been carefully studied.

We implemented and tested, for the first time, of a full three-dimensional PIC scheme with support for fully relativistic particles. Tests indicate very good performance in terms of accuracy.

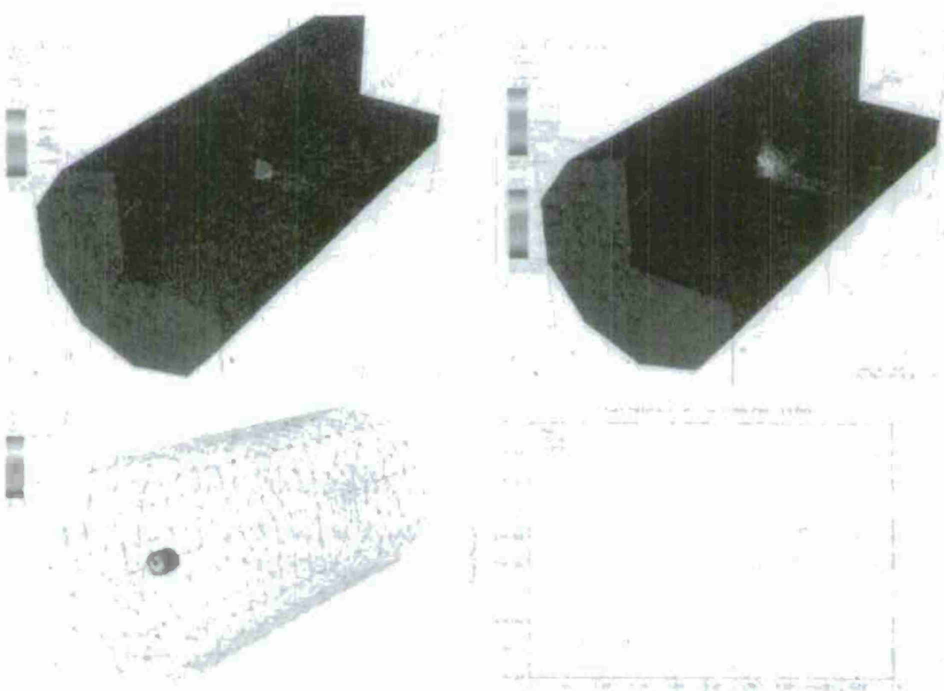
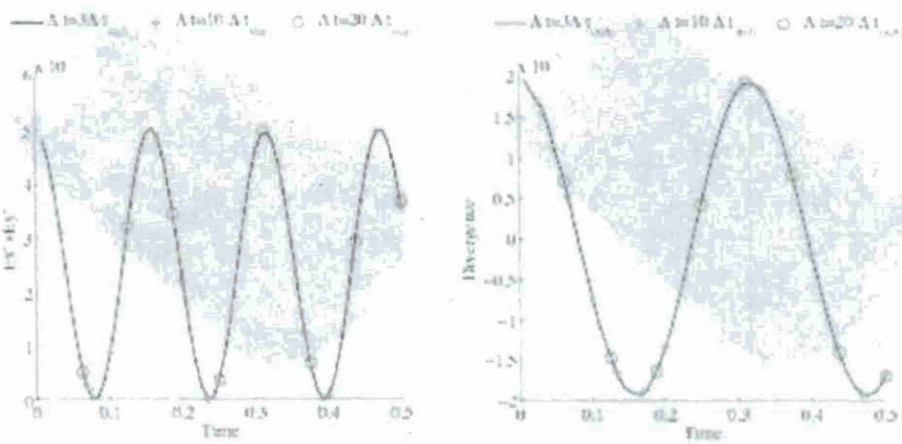


Figure 1: Examples of a three-dimensional DG based PIC simulation. The test is for the divergence of a relativistic bunch of 25k particles moving down a metallic tube, with the top figures showing the bunch of particles and the electric field, respectively. At the bottom we show the initial conditions in the grid as well as a comparison between the exact solution and the computed solution, showing excellent agreement.

Efficient time-integration techniques: A significant computational bottleneck is the temporal integration of full Maxwell-Vlasov problem on general unstructured

grids. This is not different from the pure Maxwell problem where complex geometries or poor gridding can lead to very small time-steps and a resulting significant computational cost. For the PIC model, this becomes a much more significant problem due to the high cost of the particle model and deposition. Furthermore, whereas the small cells may often the induced due to the grid, the particle dynamics do not require such small time-steps to accurately capture the important time-scales.

We have addressed this problem in two different ways. In the first one we use a mixed implicit-explicit time-stepping approach in which the Maxwell part is done implicitly, hence overcoming the small cell problem, while the particles are evolved explicitly. This also effectively deals with the important problem of divergence error control through hyperbolic cleaning techniques. Extensive tests and evaluations confirm that this is accurate and efficient and we have demonstrated a potential for a significant speedup.



Potential Energy   Divergence, $\nabla E - \rho$

Figure 2: Graphs showing the excellent accuracy of the energy and divergence with increasing time-steps using the implicit-explicit approach.

An alternative to this, and possibly a better overall solution, is the development of accurate and robust local-time stepping methods. This has first been done and demonstrated for Maxwell's equations and subsequently, using a novel extrapolation technique for the particle dynamics on the fine cells, to the full PIC problem. This is the first robust and high-order accurate local time-stepping technique for PIC problems and the computational gains of this approach are very substantial.

Particle dynamics and models: By developing a self-consistent 1.5-dimensional test case that allows us to solve it using both a PIC approach and direct Vlasov-solver techniques, we have been able to carefully analyze accuracy and

resolution requirements of the PIC methods being developed. These studies confirm that the more advanced particles shapes considered in this work are beneficial over simpler ones but also that the number of particles needed to accurately model the phase-space dynamics typically is much higher than is used in large scale applications. These studies rely on the ongoing development of a database of PIC benchmarks for benchmarking. We have, after discussions with Kirtland AFB and other key people within the kinetic plasma physics modeling community, begun the development of such a database of standard test cases and benchmarks. The beginning of the database, still in extensive development, can be seen as http://piki.tiker.net/wiki

Accurate and efficient new basis for Vlasov solvers: The direct solution of the Vlasov equation is computationally very expensive due to the high-dimensional nature. The development of efficient and compact ways of representing the velocity-dynamics is therefore of primary interest to reduce the overall cost. We have developed, carefully analyzed and implemented a novel rational basis, which is particularly well suited for the Vlasov equation. The basis is defined on all of R, allows the use of the FFT but does not require periodicity. It maintains spectral convergence and extensive analysis and tests confirm that it is superior to widely used alternatives such as Hermite functions and mapped Chebyshev functions. This basis has been implemented and used in a Vlasov solver, showing excellent results and performance which is superior to standard approaches.

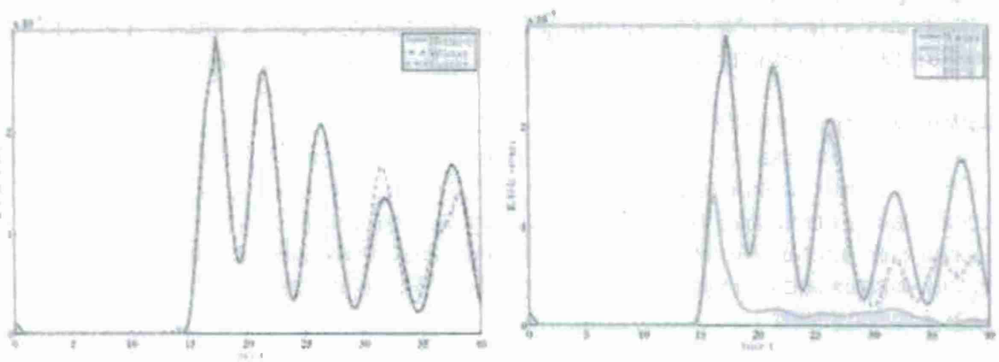


Figure 3: One the left we show results for a full Vlasov solver used to model the two-stream instability and with the velocity space represented in different ways.The new Wiener basis shows excellent long time agreement with a Hermite based method which, however, is substantially more expensive. On the right we show a direct comparison with a PIC model, illustrating convergence of the two approaches.

Acceleration and algorithm developments enabled through GPU computing: While the algorithmic changes themselves are important and valuable, the speedup offered by the use of Graphics Processing Units (GPUs) is also a substantial effort. This, however, require a detailed rethinking and reformulation

of the algorithms to fully explore this potential.

We have ported the full Maxwell solvers to GPUs, resulting in significant speedup. This has been extended to also include local time-stepping and nonlinear equations such as Euler equations. These developments have illustrated the potential for 1-2 orders of magnitude increase in computational efficiency at very limited hardware cost. It is essential to appreciate, however, that this is not achieved through simple implementation changes but requires deep changes in the algorithmic structure of the methods, e.g., whereas low order methods typically used in PIC modeling may see some benefit by using GPU based computing, high-order methods used here are much better suited for this and offer truly outstanding utilization of these new computational platforms.

Development of accurate and efficient ways to deal with shocks. When aiming to solve more complex problems, e.g., multi-scale and/or high-speed flow problems, the emergence of shocks or very steep gradients presents a significant challenge. This is relevant also for kinetic plasma physics applications in such areas as laser matter interaction or complex multiphysics where a kinetic/ continuum model is most appropriate.

For this purpose we have developed a novel, cell-local shock detector for use with discontinuous Galerkin (DG) methods. The output of this detector is a reliably scaled, element-wise smoothness estimate which is suited as a control input to a shock capture mechanism. Using an artificial viscosity in the latter role, we obtain a DG scheme for the numerical solution of nonlinear systems of conservation laws. We have thoroughly justify the detector's design and analyze and shown its performance on a number of benchmark problems.

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Personnel Supported During Duration of Grant

Akil Narayan	Brown University (PhD'09), currently postdoctoral researcher at Purdue University
Andreas Kloeckner	Brown University (PhD'10), currently postdoctoral

	researcher at NYU.
Seshu Turipathi	Brown University (PhD expected 2013).

MSc Theses directed,

1. A. Stock, *Development and application of a multirate multistep AB method to a discontinuous Galerkin method based particle-in-cell*. MSc thesis, 2009.

2. H. Riedmann, *Efficient numerical treatment of the compressible Navier-Stokes equations with nodal discontinuous Galerkin methods on graphics processors*. MSc thesis, 2009.

Publications

1. H. Haddar and J.S. Hesthaven (Eds.), *Proceedings of the 7th International Conference on Mathematical and Numerical Aspects of Waves (WAVES'05)*, J. Comp. Appl. Math. **204**(2), July 2007.
2. J. S. Hesthaven and R. M. Kirby, 2008, *Filtering in Legendre Spectral Methods*, Math. Comp. **77**(263), 1425-1452.
3. J.S. Hesthaven and T. Warburton, 2008, *Nodal Discontinuous Galerkin Methods: Algorithms, Analysis, and Applications*. Springer Texts in Applied Mathematics **54**, Springer Verlag, New York. XIV+500 pages.
4. G. Jacobs and J.S. Hesthaven, 2009, *Implicit-explicit time integration of a high-order particle-in-cell method with hyperbolic divergence cleaning*, Comput. Phys. Comm. **180,** 1760-1767.

5. A. Kloeckner, T. Warburton, J. Bridge, and J.S. Hesthaven, 2009, *Nodal discontinuous Galerkin methods on graphics processors*, J. Comput. Phys. **228**, 7863-7882.

6. G. J. Gassner, F. Lorcher, C.-D. Munz, and J. S. Hesthaven, 2009, *Polymorphic Nodal Elements and their Application in Discontinuous Galerkin Methods*, J. Comput. Phys. **228**, 1573-1590.

7. A.C. Narayan and J.S. Hesthaven, 2009, *A generalization of the Wiener rational basis functions on infinite intervals. Part I - Derivation and properties*, Math. Comp. - to appear.
8. A.C. Narayan and J.S. Hesthaven, 2009, *Computation of connection coefficients and measure modifications for orthogonal polynomials*, BIT – submitted.
9. A.C. Narayan and J.S. Hesthaven, 2009, *A generalization of the Wiener rational basis functions on infinite intervals. Part II – Numerical investigations*, J. Comput. Appl. Math. – submitted.
10. A. Kloeckner, N.Pinto, Y. Lee, B. Catanzaro, P. Ivanov, and A Fashi,

2010, *PyCUDA: Run-Time Code Generation for High-Performance Computing.* J. Parallel Comput. – to appear.

11. A. Kloecker, T. Warburton, and J.S. Hesthaven, 2010, *Viscous shock capturing in a time-explicit discontinuous Galerkin method*, Math. Model. Nat. Phenom. - to appear.
12. A. Kloeckner, T. Warburton and J.S. Hesthaven, 2010, *Solving Wave Equations on Unstructured Geometries,* GPU Computing Gems **2**, 2011 – to appear.

Honors & Awards Received

Alfred P Sloan research fellow – 2000

Manning Assistant Professorship, Brown University – 2001

NSF Career Award, NSF – 2002

Philip J Bray Award for teaching excellence in the sciences Brown University – 2004

AFRL Point of Contact

Kirtland AFRL research team on PIC. Meeting with M Bettencourt and K Cartwright during the *International Conference on Numerical Simulation of Plasma (ICNSP)*, Oct 8-12, 2007, Austin, TX. Discussions have been ongoing and continued during AFOSR annual meetings as well as through email exchanges.

Transitions — None

New Discoveries – None